Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 2/14/2017 4:48:57 PM
To: Sun, Mei [msun8@uncc.edu]; Detlef Knappe [knappe@ncsu.edu]
CC: Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: RE: FW: Chemical Structures

If it is easy to change the SI lets do it. If it is not, it is really not a big deal. Plus we have not standard to confirm which is correct. Could be both. Paul Resnick seems to think the branched isomers are more likely.

Mark

From: Sun, Mei [mailto:msun8@uncc.edu]
Sent: Tuesday, February 14, 2017 10:10 AM
To: Detlef Knappe <knappe@ncsu.edu>
Cc: Strynar, Mark <Strynar.Mark@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>
Subject: Re: FW: Chemical Structures

Sorry for the mistake... if updating the SI is not too much trouble, I'd say let's try it.

Mei Sun

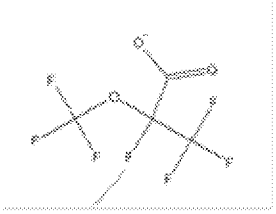
Assistant Professor
Department of Civil and Environmental Engineering
University of North Carolina at Charlotte
Energy Production and Infrastructure Center 3163
9201 University City Blvd | Charlotte, NC 28223
Phone: 704-687-1723 | Fax: 704-687-0957
Website: https://coefs.uncc.edu/msun8/

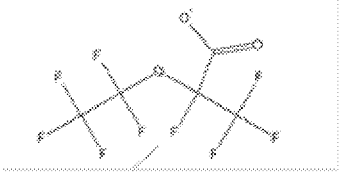
On Tue, Feb 14, 2017 at 7:57 AM, Detlef Knappe <knappe@ncsu.edu> wrote:

> I should have noticed that, too... Should we explore an erratum? Since it involves the SI, updating the SI may be possible even without an erratum.

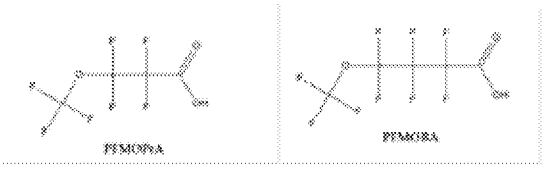
On 2/14/17 7:44 AM, Strynar, Mark wrote:

> > In our paper Strynar et al., 2015 we proposed these structures as below: (Figure S7). These are the ones Paul suggests are more likely.





In Sun et al., 2016 we showed them different (Figure S1).



I should have noted this in the SI.

The QTOF can distinguish between the two as the likely breaking point is at the ether oxygen. We would get different fragments for the PFMOBA, not the PFMOPrA.

Mark

From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Monday, February 13, 2017 8:13 AM

To: Strynar, Mark <Strynar.Mark@epa.gov>; Lindstrom, Andrew <Lindstrom.Andrew@epa.gov>; msun8@uncc.edu
Subject: Re: FW: Chemical Structures

Interesting... But Synquest does make the non-branched compounds we are showing (see first two compounds in the attached). Would QTOF work be able to distinguish between linear and branched?

On 2/13/17 7:22 AM, Strynar, Mark wrote:

> FYI,
>
> I will need to take a closer look at his comment later.
>
> Mark

From: Paul [mailto: **Personal Matters / Ex. 6**
Sent: Saturday, February 11, 2017 6:30 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: Chemical Structures

Mark:

Just finishing looking at Env. Sci. & Tech. Letters 2016 3 (12) 415 for use as a reference.

Legacy and Emerging Perfluoroalkyl Substances Are Important

Drinking Water Contaminants in the Cape Fear River Watershed of

North Carolina

Mei Sun,*,†,‡ Elisa Arevalo,‡ Mark Strynar,§ Andrew Lindstrom,§ Michael Richardson,‖ Ben Kearns,‖

Adam Pickett,⊥ Chris Smith,# and Detlef R. U. Knappe‡

†Department of Civil and Environmental Engineering, University of North Carolina at Charlotte, Charlotte, North Carolina 28223,

United States

‡Department of Civil, Construction, and Environmental Engineering, North Carolina State University, Raleigh, North Carolina

27695, United States

§National Exposure Research Laboratory, U.S. Environmental Protection Agency Research, Triangle Park, North Carolina 27711,

United States

∥Cape Fear Public Utility Authority, Wilmington, North Carolina 28403, United States

⊥Town of Pittsboro, Pittsboro, North Carolina 27312, United States

#Fayetteville Public Works Commission, Fayetteville, North Carolina 28301, United States

I believe that the structural assignments for PFMOBA [$CF_3OCF_2CF_2CF_2COOH$] and PFMOPrA [$CF_3OCF_2CF_2COOH$] are most likely incorrect.

More reasonably the correct structures are isomers $CF_3CF_2OCF(CF_3)COOH$ and $CF_3OCF(CF_3)COOH$ respectively. I doubt that the MS/MS could tell the isomers apart.

If you want to discuss this further please call me. (703) 567-6832.

Best regards,

Paul

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Detlef Knappe
Professor
319-E Mann Hall
Department of Civil, Construction, and Environmental Engineering
North Carolina State University
Campus Box 7908
Raleigh, NC 27695-7908

Phone: 919-515-8791
Fax: 919-515-7908
E-mail: knappe@ncsu.edu
Web page: http://knappelab.wordpress.ncsu.edu/

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Detlef Knappe
Professor
319-E Mann Hall
Department of Civil, Construction, and Environmental Engineering
North Carolina State University
Campus Box 7908
Raleigh, NC 27695-7908

Phone: 919-515-8791
Fax: 919-515-7908
E-mail: knappe@ncsu.edu
Web page: http://knappelab.wordpress.ncsu.edu/